Author index

Adiraj,M. 1005
Aikawa,J.-i. 869
Albert,A. 885
Aldape,R.A. 173
Alesker,V. 1103
Alexandrov,N.N. 727
Alkorta,I. 573
Almashanu,S. 803
Almo,S.C. 773
Arcila,P. 283
Argos,P. 133, 249, 471, 1121
Arias,A.R.L. 1173
Arnold,F.H. 77
Atkins,W.M. 291
Avery,B. 895
Ayvazian,L. 707
Bagossi,P. 997
Baker,C.B. 849
Baker,K.C. 525
Baldwin,J. 189
Barbosa,J.A.R.G. 591
Barr,P.J. 585
Battistoni,A. 323
Bautista,D.L. 1029
Bedarkar,S. 631
Bedouelle,H. 231
Beer,H.D. 507
Beiboer,S.H.W. 345
Bennett,W.F. 283
Beppu,T. 869
Berleau,L.T. 283
Bernhagen,J. 631
Bhat,S.P. 713
Birch,A. 365
Bizebard,T. 181
Blaszczyk-Thurin,M. 447
Blättler,W.A. 895
Blöcker,H. 931
Blondel,A. 231
Blundell,T.J. 849
Blundell,T.L. 885
Board,P.G. 327
Bohr,J. 733
Bontems,F. 949
Bork,P. 725
Brasseur,R. 317
Breed,J. 161
Breitling,F. 203
Bridges,A. 365
Brissinck,J. 299
Brodbeck,W. 1143
Brooks III,C.L. 657
Brown,E.M. 43
Brunak,S. 733
Bucala,R. 631
Buehler,F.U. 499
Bülow,L. 1051
Burbage,C. 371, 913
Canaan,S. 1225
Cao,B. 15
Capalbo,L. 1191
Carr,M.T. 323
Carter,P. 617
Carver,J.A. 1021
Casari,G. 941
Chan,S.L. 977
Chandler,J. 371, 913
Chang,C.-C. 1165
Chang,Y.-T. 755
Chapus,C. 707
Chayen,N.E. 927
Chelvanayagam,G. 1151
Chemeris,V.V. 195
Chen,H. 499
Chen,J.M. 43
Chen,Q. 545
Cheng,D. 713
Cheng,Y.-S.E. 997
Chiche,L. 959
Chirgadze,Y.N. 745
Chirn,G.W. 381
Chou,C.-C. 623
Ciaramella,M. 1191
Cinquina,C. 631
Claeyssens,M. 691
Clark,N.S. 877
Clausen,I.G. 519
Co,M.S. 447
Cockburn,W. 1211
Collins,R.A. 1203
Connerton,I.F. 525
Cook,S. 895
Cook,W.J. 623
Cox,R.C. 345
Crenon,I. 707
Cummings,N.J. 525
Da Silva,N.A. 1197
Dabrowski,M.J. 291
Dahl,S.G. 149
Danson,M.J. 629
Davenport,R.C. 61
Davies,J. 531
de Filippis,V. 439
de Jong,W.W. 1021
De Meyts,P. 1011
De Reggi,M. 949
De Wolf,E. 1011
DeBolt,S.E. 637
DeCenzo,M.T. 173
Dekker,N. 345
Delbaere,L.T.J. 539
dePrat-Gay,G. 843
Derewenda,U. 789
Derewenda,Z.S. 789
Desideri,A. 323
Desmadril,M. 181
Dhanaraj,V. 885
Dietze,E.C. 291
Doak,D.G. 161
Dodd,I. 877
Doi,T. 307
Dolgikh,D.A. 195
Dorner,F. 921
Doughty,S.W. 493
Drueckes,P. 701
Dübel,S. 203
Dumas, C. 181
Dupuis,L. 1225
Earhart,C.F. 239
Earnshaw,J.C. 1043
Easteal,S. 1151
Edvardsen,Ø. 149
Efremov,R.G. 253
Eguchi,N. 1067
Eibl,J. 921
Eijsink,V.G.H. 1181
Eisenhaber,F. 1121
Emoto,T. 1173
Faiman,G.A. 315
Falconi,M. 323
Fauman,E.B. 69
Fedorov,A.A. 773
Fedorov,A.N. 195
Feng,M.-H. 977
Finer-Moore,J.S. 69
Finkelstein,A.V. 387, 399
Fischer,B.E. 921
Fitzpatrick,P.A. 585
Folcarelli,S. 323
Ford,C. 499
Fothergill-Gilmore,L.A. 1203
Francescutti,D. 189
Frankel,A. 371
Frankel,A.E. 913
Frigerio,F. 439
Frishman,D. 133
Fu,T. 913
Futer,O. 173
Gabrielian,A.E. 195
Gao,X. 1151
Gardner,S.P. 1063
Garratt,R.C. 591
Gauthier,F. 987
Gendler,I. 803
Georgiou,G. 239
Gharib,B. 949
Gill,R. 1011
Go,N. 1083
Gong,X. 797
Gore, M.G. 877
Gotter, S. 203
Grandi,G. 439
Granon,S. 707
Grassy,G. 959
Green,J. 849
Grillberger,L. 921
Grötzinger,J. 1011
Grundström,G. 1051
Gu-Tian,X. 555
Guidi-Rontani,C. 611
Guild,B.C. 895
Guruprasad,K. 849
Hadar,R. 803
Haiech,J. 959
Hakala,J.M.L. 143
Han,H. 479
Hansen,J.E. 733
Harrison,R.W. 333, 679
Haruki,M. 857
Hayaishi,O. 1067
Hedstrom,L. 85
Henke,C. 365
Henrissat,B. 725
Henry,A.H. 895
Hicks,L. 353
Hiraga,K. 425, 433
Hirst,J.D. 657
Hodges,R.S. 353, 1029
Hoffee,M. 895
Holliger,P. 299
Holmberg,N. 1051
Holmquist,M. 519
Horinouchi,S. 869
Hornischer, K. 931
Horovitz,A. 315
Hough,D.W. 629
Huang,P.C. 1165
Huber,C.P. 977
Hult,K. 519
Imaizumi,A. 101
Imanishi,T. 307
Imoto, T. 95, 461
Irvin,R.T. 1029
Ishii,K. 101
Jacoby,E. 113
Jaenicke,R. 1021
Jakobsen,I.B. 1151
Janocha,E. 213
Jarrett,B.P. 173
Jeanteur,D. 857
Jeltsch,A. 413
Johnson,K.S. 1043
Jones,T.A. 691
Joseph-McCarthy,D. 773
Kamimura,T. 101
Kaminogawa,S. 467
Kanaya,S. 857
Kanehisa,M. 27
Kanesaki,M. 101
Kantrowitz,E.K. 1233
Kashiwagi,T. 857
Katayanagi,K. 857
Kato,H.1083
Katti,S.B. 1005
Kay,C.M. 353, 789
Kelley,L.A. 1063
Kellis Jr,J.T. 1197
Kelly,S.M. 1203
Kerfelec, B. 707
Kerr,I.D. 161
Keyt,B.A. 283
Kieber-Emmons,T. 447
King,G. 43
Kipriyanaov,S.M. 203
Kirpichnikov,M.P. 195
Kirsch,J.F. 1055
Kleywegt,G.J. 691
Kodama,T. 307
Kohima,Y. 1173
Koivula,A. 691
Kojima,S. 1241
Kolinski,A. 5
Kollman,P.A. 273
Koskinen, A.M. 143
Kroemer,R.T. 493, 1135
Kropshofer,H. 203
Krüger,P. 113
Kubodera,H, 1067
Kuhn,J. 803
Kumuagai,I. 1211
Kurasaki,M. 1173
Kuttner-Kondo,L. 1143
Kwon,W.S. 1197
Lai,L. 479
Lallemand,J.-Y. 949
Lambert,J.M. 895
Lamerdin,J.A. 781
Landgraf,R. 603
Lang,S. 365
Lanio,T. 1005
Le,T.H. 181
Lebras,G. 181
Lee,L. 189
Lee,M.S. 15
Lee,S.-H. 467
Lee,T.Y. 381
Lentz,B.R. 545
Li,S. 479
Li,V. 499, 905, 1211
Lim,C. 977
Lindvall, M. 143
Lins,L. 317
Little,M. 203
Livingston,D.J. 173
Lobb,L. 1233
Loew,G.H. 573, 755
Lolis,E. 631
Lord,S.T. 545
Lund,O. 733
Lunt,G.G. 51
Maeda,Y. 95, 461
Magyar,C. 663
Mahoney,W. 1043
Margarit,I. 439
Markman,O. 1233
Marr,T.G. 381

Martinelle,M. 519
Mase,T. 789
Masuda,K. 101
Matsuda,K. 1083
Matsuzawa,H. 467
May,A.C.W. 1093
McCafferty,J. 1043
McCarthy,J.E.G. 507
McDowell,K. 849
McElhaney,R.N. 789
McElver,J. 1055
McMullen,T. 789
Medof,M.E. 1143
Meijer,P.-J. 1051
Mendenhall,J. 239
Mevissen,H.Th 127
Middelhoven,P.J. 1181
Milpetz,F. 249
Minagawa,E. 467
Minard,P. 181
Mitterer,A. 921
Miura,K.-i. 1241
Miyoshi,K. 1241
Mizuguchi,K. 1083
Monera,O.D. 353
Moracci,M. 1191
Moreau,T. 987
Morikawa,K. 857
Morris,A.J. 61
Morse,R.J. 69
Mossakowska,D.E. 877
Mozo-Villarias,A. 265
Muirhead,H. 1203
Mundt,W. 921
Murali,R. 447
Murcko,M.A. 173, 767
Murgolo,N.J. 623
Murray-Rust,J. 1011
Mutus,B. 189
Nagabhushan,T.L. 623
Nagaraj,R. 1219
Nagel,R.J. 849
Nageotte,R. 231
Nakahima,N. 1067
Nakamura,H. 307
Nandagopal,K. 781
Nandy,P. 713
Narula,S.K. 623
Navolotskaya,E.V. 195
Nguyen,H.V. 283
Nicolini,L. 323
Nishikawa,A. 307
Nishioka,T. 1083
Nishiyama,M. 869
Niyogi,S.K. 781
Nogarotto,R. 439
Nugent,P.G. 885
Nussinov,R. 1103
Oda,J. 1083
Ohta,T. 467
Ohtsuka,E. 101
Oikawa,K. 789
Oikawa,S. 1173
Okabe,M. 1173
Olszewski,K.A. 5
Ornstein,R.L. 485, 567, 721
Oroszlan,S. 997
Orprayoon,P. 885
Ortells,M.O. 51
Otto,B. 905
Owen,M.R.L. 1211
Packman,L.C. 559
Pan,C. 603
Panda,T. 499
Park,S.T. 173
Park,Y.-N. 869
Parker,M.W. 327
Parsons,H.L. 1043
Pascarella,S.249
Patard,L. 949
Patkar,S. 519
Paulsen,M.D. 567
Pearl,L. 629
Pearson,L. 603
Pedersen,J.T. 895
Pemberton,P.A. 585
Perez-Pons,J.A. 265
Petithory,J.R. 1055
Petrenko,V.A. 797
Petro,M. 623
Pingoud,A. 413, 1005
Pitts,J. 1011
Pitts,J.E. 885
Poetschke,H.L. 239
Polticelli,F. 323
Prasad,L. 539
Presta,L.G. 617
Price,N.C. 1203
Querol,E. 265
Quinn,T. 797
Ralston,G.B. 223
Ramanathan,L. 623
Ramjee,M.K. 1055
Rao,B.G. 767
Rees,A.R. 895
Reese,M.G. 733
Reichelt,J. 833
Reilly,P.J. 499
Reinikainen,T. 691
Reiter,M. 921
Reva,B.A. 387, 399
Richards,W.G. 493, 1135
Ridgway,J.B.B. 617
Riechmann,L. 531
Riley,L.G. 223
Rivière,M. 1225
Roberts,R.M. 849
Robinson,A.J. 493
Robinson,J.A. 365
Roguska,M.A. 895
Roja,C.M. 895
Röper,D. 113
Rosato,N. 323
Rossi,M. 1191
Rossjohn,J. 327
Rotilio,G. 323
Rouvinen,J. 691
Ruohenen,L. 691
Russell,R.B. 107
Russell,R.J.M. 629
Rutter,W.J. 85
Saldanha,J.W. 591
Sander,C. 941
Sanejouand,Y.H. 671
Sankararamakrishnan,R. 161
Sansom,M.S.P. 161
Santi,D.V. 69
Schäfer,T. 905
Schinzel,R. 701
Schlitter,J. 113
Schlokat,U. 921
Schmid,R.D. 507
Schneider,G. 833
Schneider,J. 213
Schomburg,D. 507, 833, 905
Schuchhardt,J. 833
Schueler,P.A. 1043
Schulz,A. 1005
Scott,S.-P. , 333
Searle,M.S. 559
Sehl,L.C. 283
Sekiya,T. 1067
Selent,U. 1005
Serpersu,E.H. 781
Sha,Y. 539
Shapiro,B.A. 381
Shasha,D. 381
Shoham,M. 1143
Sigman,D.S. 603
Sitay,A. 713
Skolnick,J. 5, 637
Skolnick,J. 657
Smith,G.P. 797
Smith,R.A.G. 877
Sobotta,T. 413
Sönnichsen,R.D. 353
Späth,J. 365
Srinivasan,A. 713
Stathopoulos,C. 239
Stec,B. 1233
Steffens,G.J. 213
Stella,L. 323
Stephens,D.L. 239
Steplewski,Z. 447
Sternberg,M.J.E. 107
Stojanoff,V. 1233
Stoven,V. 949
Stroud,R.M. 69
Stuart,F. 365
Sugiyama,T. 101
Sun,H.-W. 631
Sun,Y.-C. 273
Sutcliffe,M.J. 1063
Sutton,C. 603
Suzuki,Y. 101
Svendsen,A. 519
Swope,M. 631
Sylte,I. 149
Szafranska ,B. 849
Szardenings,M. 691
Szilágyi,A. 663
Tabolina,O.Y. 745
Tadaki,D.K. 781
Tagge,E. 371, 913
Taguchi,H. 467
Takeuchi,K. 789
Talmud,P. 317
Tanaka, J.C. 333
Tanaka,T. 307, 1067
Tanaka,Y. 307
Tang,Y. 479
Taylor,G.L. 629
Taylor,M.A.J. 525
Teeri,T.T. 691
Teeter,M.M. 1233
Teleman,O. 691
Thennarasu,S. 1219
Thielemans,K. 299
Thomas,D.J. 941
Toh,H. 1067
Tolan,D.R. 61
Tomii,K. 27
Tougard,P. 181
Tözsér,J. 997
Tripet,B. 1029
Trotta,P.P. 623
Tuñón,M.-A. 525
Ueda,T. 95, 461
Urade,Y. 1067
Ursø,B. 1011
Uversky,V.N. 195
Vakser,I.A. 37, 741
Valkeajärvi,A. 691
van den Berg,B. 345, 1181
Veenstra,D.L. 273
Veltman,O.R. 1181
Venekei,I. 85
Venema,G. 1181
Verger,R. 1225
Vergoten,G. 253
Verheij,H.M. 345
Verma,C. 1011
Vieth,M. 657
Villmann,C. 905
Vingron,M. 127
Vriend,G. 1181
Wallach,B. 1011
Walter,L.J. 623
Walther, D. 471
Wang,J.T.L. 381
Wang,Y. 479
Waschütza,G. 905
Weber,I.T. 333, 679
Weber,S.C. 1055
Weiss,A.S. 223
Wende,W. 1005
Wenz,C. 1005
Werten,P.J.L. 1021
Westerink,M.A.J. 447
Whitelam,G.C. 1211
Wicker-Planquart,C. 1225
Wilce,M.C.J. 327
Williams,D.H. 559
Williams,R.L. 299
Willingham,M. 371, 913
Wilsher,J. 885
Wilton,J. 1043
Winter,G. 299
Wnendt,S. 213
Wohlfahrt,G. 507
Wolfson,H.J. 1103
Wollmer,A. 113, 1011
Wong,D.T. 585
Wong,W.Y. 1029
Wood,S. 1011
Worboys,K.A. 525
Wrede,P. 833
Xiang,J. 539
Xiang,Y. 977
Xie,S. 849
Yamada,H. 461
Yamaguchi,S. 789
Yamano,A. 1233
Yamasaki,F. 1173
Yasri,A. 959
Yi,X. 555
Yon,J.M. 181
Yoshimura,E. 467
You,L. 77
Yu,L. 1029
Yu-Long,S. 555
Yun-Hua,W. 555
Yutani,K. 425, 433
Zakaria,H. 905
Zav'yalov,V.P. 195
Závodszky,P. 663
Zerella,R. 559
Zevodny,P.J. 623
Zheng,Y.-J. 485, 721
Zhong-Xian,H. 555

Subject index

3D_ali
updated version of database 249
8-OH-DPAT
molecular modelling of interaction with 5-hydroxytryptamine 1a receptor 149
Acetate
used for chemical rescue of mutant maltodextrin phosphorylase 701
β-Actin
secondary structure analysis of profilin–β-actin complex 1103
Active site
of linked HIV-1 proteinase dimer, effect of mutating 997
of *Taq* carboxypeptidase 467
of *Trichoderma reesei* cellobiohydrolase, site-directed mutagenesis 691
Affinity chromatography
coiled coil heterodimerization domain as fusion tag for detecting recombinant proteins and peptides 1029
Albetin
grafting blast-transforming activity of interferon 195
Aldolase
rate-determining step changed by site-directed mutagenesis 61
AMBER
for modelling metal-binding sites 931
Antibacterial peptides
derived from pardaxin 1219
Antibodies
against carbohydrates, molecular recognition of Lewis Y antigen 447
directed selection of antibody repertoires displayed on phage 1043
humanization by CDR grafting and resurfacing 895
humanization of rat monoclonal Fab against human interleukin-5 623
improving stability of camelized human V_H domains 531
knobs-into-holes engineering for designing antibody–immunoadhesin hybrid 617
towards development of multivalent antibodies 203
Antibody–antigen interaction
HyHEL-10 residues involved in 1211
site-directed mutagenesis study of 539
Antibody fragments
bispecific, cytotoxicity of 299
Antifreeze protein
directed evolution of 1051
Apolipoprotein B
molecular modelling of signal peptide 317
Aspartic proteinases
catalytic mechanism of *Rhizomucor pusillus* pepsin 869
comparative modelling of pregnancy-associated glycoproteins 849
modelling interaction of human immunodeficiency virus protease of peptide fragments 679
site-directed mutagenesis of chymosin loops 885
Aspergillus awamori
glucoamylase, thermostability of 499
ATP-binding motif
in glutathione synthetase 1083
Autocorrelation
for rational choice of parameters in molecular dynamics simulation 959
Autolysis
of thermolysin-like protease *Bacillus stearothermophilus*, factors affecting 1181

B72.3 antibody
interaction with TAG72 antigen, site-directed mutagenesis study 539
Bacillus stearothermophilus
thermolysin-like protease, factors affecting autolysis of 1181
Bacillus subtilis
neutral protease, improving thermostability of 439
Bacteriophage M13
gene V protein, stability of in GVP–MalE fusion protein 231
Baculovirus vector
cloning human gastric lipase 1225
Barnase
effect of Ile96→Ala mutation on stability 273
thermostability, effect on rate of proteolysis 1197
Binding free energy
of cytochrome P450cam interaction with substrate, estimation of 567
Biological function
grafting blast-transforming activity of interferon on to albetin 195
Blast-transforming activity
of interferon, grafting on to albetin 195
Blocks
of amino acids, as a basis for protein classification 381

C3 convertase
recognition sites for in DAF, homology modelling of 1143
Calcitonin gene-related peptide
molecular modelling of constrained analogues 143
Calmodulin
molecular dynamics simulation, autocorrelation for rational choice of parameters 959
Calycin superfamily
structural similarity of catalase 107
Carbohydrates
antibodies against, molecular recognition of Lewis Y antigen 447
Carbon tetrachloride
effect on subtilisin 485
Carboxypeptidase
Taq, active site of 467
Catalase
structural similarity to calycin superfamily 107
Catalytic mechanism
of *Rhizomucor pusillus* pepsin, site-directed mutagenesis study 869
Cathepsin B
docking of inhibitor, molecular dynamics study 977
CD4
conformational change upon binding human immunodeficiency virus gp120 671
Cell surface
Escherichia coli, displaying β-lactamase on 239
Charge clusters
on surface of γ-crystallin protein 745
Che Y
secondary structure analysis 1103
Chemical rescue
of mutant maltodextrin phosphorylase by acetate 701
4-Chlorobenzoyl CoA dehalogenase
mechanism of dehalogenation by [Forum] 721
Chloroform
selection of chloroform-resistant filamentous phage from landscape library 797
Chymosin
site-directed mutagenesis of loops 885
Circular dichroism
compared with nuclear magnetic resonance for estimating secondary structure 15
Classification
of modular proteins [Forum] 725
Cluster analysis
of NMR-derived protein structures, automated method for [Protocol] 1063
Coiled coil
as fusion tag for detecting recombinant proteins and peptides 1029
multiple stranded, control of formation of 353
Collagen
collagen-like domain from macrophage scavenger receptor binds acetylated LDL *in vitro* 307
molecular modelling of bovine type I microfibril 43
Comparative modelling
of pregnancy-associated glycoproteins 849
Complement receptor 1
human, folding of SCR1–3 domains 877
Complementarity-determining region
residues involved in antibody–antigen interaction 539
Crambin
recombinant, produced from synthetic gene 1233
Crystallin
α- and αA^{ins}-crystallins compared 713
βA3 and βA1, role of N-terminal extension 1021
γ-crystallin, charge clusters on protein surface 745

Crystallization
of proteins: preventing heterogeneous nucleation [Protocol] 927
Cucurbita maxima
trypsin inhibitor I, synthesis as fusion protein 1241
Cyclic nucleotides
predicted interaction with ion channels 333
Cysteine proteinases
molecular dynamics study of cathepsin B inhibitor docking 977
preventing autoprocessing of papaya proteinase IV proenzyme 525
Cysteine residues
in *Escherichia coli* tryptophan synthase, role in enzyme function 433
role in stability of *Escherichia coli* tryptophan synthase 425
unpaired, in tissue-type plasminogen activator, locating 283
Cytochrome b_5
interaction with cytochrome *c*, site-directed mutagenesis study of 555
Cytochrome *c*
interaction with cytochrome b_5, site-directed mutagenesis study of 555
Cytochrome P450cam
interaction with substrate, estimation of binding free energy 567
Cytochrome P450choP
homology modelling of 755
Cytotoxicity
of diabodies 299

Databases
3D_ali, updated version of 249
database of site-directed thermostability mutants 265
Decay-accelerating factor
human, homology modelling of 1143
Dehalogenation
by 4-chlorobenzoyl CoA dehalogenase, mechanism of [Forum] 721
Diabodies
cytotoxicity of 299
Dimerization domain
transplantation 223
Directed evolution
of antifreeze protein 1051
of subtilisin E in *Bacillus subtilis* 77
Directed selection
of antibody repertoires displayed on phage 1043
Distance distributions
for structure prediction 733
Disulfide bond
engineering in interferon-γ 905
insertion into *Penicillium camembertii* lipase, effect on thermostability 789
DNA cleavage
site-specific, semisynthetic scission reagent derived from Trp repressor 603
DNA methyltransferase
*Eco*RV, structure prediction 413
Docking
of cathepsin B inhibitor, molecular dynamics study 977
Docking algorithm
to study role of main-chain complementarity in ligand–receptor interaction 741
Double-mutant cycles
choice of reference mutant states, [Letter] 315
Dynamic light scattering
study of macrophage migration inhibitory factor 631

***Eco*RV**
DNA methyltransferase, structure prediction 413
substrate specificity, altering by site-directed mutagenesis 1005
Endopeptidases
glutamate-specific, molecular modelling of active site 591
Energy minimization
modelling interaction of human immunodeficiency virus protease with peptide fragments 679
targeted, for simulation of T⟷R transition 113
Enterotoxin
as basis for model of nicotinic acetylcholine receptor transmembrane domain 51
Environmental profile
algorithm for recognizing transmembrane domains in integral membrane proteins 253

Enzymes
thermostability of [Forum] 629
Epidermal growth factor
role of Leu15 in ligand–receptor interaction 781
Epidermolytic toxins
molecular modelling of active site 591
Escherichia coli
displaying β-lactamase on cell surface 239
efficient production of SLPI protease inhibitor C-terminal domain in 101
glutamine synthetase, 'salting out' is abolished by single amino acid substitution 291
ribonuclease HI, site-directed mutagenesis and X-ray crystallography 857
thermostable 3-isopropylmalate dehydrogenase, homology modelling of 663
tryptophan synthase, role of cysteine residues in enzyme function 433
tryptophan synthase, role of cysteine residues in stability 425
Ester bonds
hydrolysis by lipases, identifying residues important in catalysis 507
Exotoxin A
Pseudomonas aeruginosa, for delivering large proteins into cells 611

Ferredoxin
peptide fragment, forms native-like β-hairpin 559
Fibrinolysis
chimeric derivatives of prourokinase with thrombin-inhibitory potential 213
Filamentous phage
selection of chloroform-resistant viruses from landscape library 797
FITSITE
algorithm for modelling metal-binding sites 931
FK506-binding protein
effects of active site mutation 173
FKBP12
effects of active site mutation 173
Fluorescent label
introducing into prothrombin 545
c-Fos
leucine zipper dimerization domain 223
Free energy
of unfolding of wild type and mutant barnase 273
Free energy perturbation
of HIV-1 protease inhibitors 767
Freezing tolerance
Escherichia coli, relationship with NaCl tolerance 1051
Functional group mapping
of RNase A 773
Fusion protein
crambin–maltose-binding protein 1233
GVP–MalE, stability of gene V protein in 231
Fusion tag
affinity chromatography, for detecting recombinant proteins and peptides 1029
Fusion toxin
ricin–IL-2 913
Fv fragment
inhibits cytokine binding to interferon-γ receptor 365
single chain, fusion with streptavidin core 203

Galactose binding
by ricin, mutational analysis of 371
Gene V protein
bacteriophage M13, stability of in GVP–MalE fusion protein 231
Global minimum
in ligand–receptor interaction, identifying using long-distance potentials 37
Globin fold
comparison of proteins with 727
Glucoamylase
Aspergillus awamori, thermostability of 499
Glutamine synthetase
Escherichia coli, 'salting out' is abolished by single amino acid substitution 291
Glutathione reductase
effect of peroxynitrite modification 189
Glutathione synthetase
structure comparison with other proteins 1083

Glutathione transferases
theta class, sequence comparison 327
β-Glycosidase
Sulfolobus solfataricus, identifying residues essential for catalysis 1191

Haemoglobin
directed selection of anti-HbF antibodies 1043
Haemolysis
by peptides derived from pardaxin 1219
β-Hairpin
native-like, is formed in ferredoxin peptide fragment 559
α-Helices
control of formation of multiple stranded coiled coils 353
rigidity of, effect of Glu→Ala mutations 499
stability of, role of side-chain–side-chain interaction 471
Heterodimerization
of antibody heavy chains by knobs-into-holes engineering 617
Heterodimerization domain
coiled coil, as fusion tag for detecting recombinant proteins and peptides 1029
HLA-A
homology modelling 1151
Homology modelling
for interleukin-7 structure prediction 493
of cytochrome P450choP 755
of HLA-A 1151
of human decay-accelerating factor 1143
of interleukin-7 complex with receptor 1135
of lithostathine 949
of maspin 585
of rat kallikrein rK9 987
Human immunodeficiency virus
effect of mutating linked HIV-1 proteinase dimer active site 997
gp120, conformational change in CD4 upon binding 671
HIV-1 protease, binding of inhibitors to 767
protease, modelling interaction with peptide fragments 679
Humanization
of antibodies by CDR grafting and resurfacing 895
of rat monoclonal Fab against human interleukin-5 623
Humicola lanuginosa
lipase, effect of site-directed mutagenesis on substrate specificity 519
Hydration shell
structure, for defining hydrophobic patches on protein surface 1121
Hydrogen bonding
long-range, predicting from amino acid sequence 133
Hydrolysis
of ester bonds, by lipases, identifying residues important in catalysis 507
Hydrophobic interactions
contribution to thermostability of *Bacillus subtilis* neutral protease 439
Hydrophobic patches
on protein surface, defining from hydration shell structure 1121
5-Hydroxytryptamine 1a receptor
molecular modelling of interaction with UH-301 and 8-OH-DPAT 149
HyHEL-10
residues involved in antibody–antigen interaction 1211

Immunoadhesin
knobs-into-holes engineering for designing antibody–immunoadhesin hybrid 617
Immunoglobulin G
reduced, renaturation *in vitro* 95
Insect cells
expression of human gastric lipase in 1225
Insulin
simulation of T⟷R transition in hexamer 113
Insulin-like growth factor
site-directed mutagenesis, effect on receptor binding 1011
Integral membrane proteins
algorithm for recognizing transmembrane domains 253
Interferon
grafting blast-transforming activity on to albetin 195
Interferon-γ
engineering disulfide bonds to improve thermostability 905
Interferon-γ receptor
monoclonal antibodies Fv fragment inhibits cytokine binding 365
Interleukin-2
ricin–IL-2 fusion toxin 913
Interleukin-5
human, humanization of rat monoclonal Fab against 623
Interleukin-7
homology modelling of complex with receptor 1135
structure prediction by homology modelling 493
Internalization
delivery of large proteins into cells by *Pseudomonas aeruginosa* exotoxin A 611
Interspecific hybrids
construction of bacterial luciferase β-subunit hybrids 803
Inverse folding
evaluation of knowledge-based atomic level mean force potentials 637
mean force-field calculation for predicting stability of mutant proteins 479
Inverse refinement
evaluation of knowledge-based atomic level mean force potentials 637
Invertase
molecular modelling of yeast signal peptide 317
Ion channels
model of nicotinic acetylcholine receptor transmembrane domain 51
predicted interaction with cyclic nucleotides 333
Staphylococcus aureus δ-toxin, molecular modelling of 161
3-Isopropylmalate dehydrogenase
Escherichia coli thermostable, homology modelling of 663

c-Jun
transplantation of leucine zipper dimerization domain 223

Kallikrein
rat rK9, homology modelling 987
Knobs-into-holes engineering
for designing antibody–immunoadhesin hybrid 617
Kohonen algorithm
neural network, for protein structure classification 833

β-Lactamase
displaying on *Escherichia coli* cell surface 239
Landscape library
selection of chloroform-resistant filamentous phage from 797
Lattice model
of protein folding 5, 387, 399
Lectin-binding sites
in ricin 371
Leucine zipper
predicting from sequence 657
transplantation of c-Fos/c-Jun dimerization domain 223
Lewis antigens
molecular recognition of Lewis Y antigen by monoclonal antibodies 447
Ligand–receptor interaction
3D model of δ-opioid receptor 573
epidermal growth factor, role of Leu15 781
identifying global minimum using long-distance potentials 37
molecular modelling of 149
role of main-chain complementarity 741
Lipase
human gastric, expression in insect cells 1225
Humicola lanuginosa, effect of site-directed mutagenesis on substrate specificity 519
pancreatic, function of C-terminal domain 707
Penicillium camembertii, thermostability, effect of inserting disulfide bond 789
Rhizopus oryzae, identifying residues important in catalysis 507
Lipocalins
molecular evolution of [Review] 1067
Lithostathine
homology modelling and NMR spectroscopy 949
Long-distance potentials
for identifying global minimum in ligand–receptor interaction 37
Loops
in chymosin, site-directed mutagenesis of 885
Low density lipoprotein
collagen-like domain derived from macrophage scavenger receptor binds acetylated LDL *in vitro* 307
Luciferase
bacterial, construction of β-subunit hybrids 803
Lysozyme
reduced, effect of additives on renaturation of 461

Macrophage migration inhibitory factor
X-ray diffraction study of 631
Macrophage scavenger receptor
derived collagen-like domain binds acetylated LDL *in vitro* 307
Major histocompatibility complex
structure comparison of MHC class I molecules 1151
Maltodextrin phosphorylase
mutant, chemical rescue by acetate 701
Maltose-binding protein
stability of gene V protein in GVP–MalE fusion protein 231
Maspin
homology modelling of 585
Mean force potentials
atomic level knowledge-based, evaluation of 637
Mean force-field
calculation for predicting stability of mutant proteins 479
Metal binding
by metallothionein, semi-empirical simulation of Zn/Cd binding site preference 1165
Metal-binding sites
modelling using FITSITE 931
Metallothionein
α-fragment, independent self-assembly 1173
metal binding, semi-empirical simulation of Zn/Cd binding site preference 1165
Microbatch crystallization
method for preventing heterogeneous nucleation [Protocol] 927
Modelling
of metal-binding sites, using FITSITE 931
Modular proteins
classification of [Forum] 725
Molecular dynamics
rational choice of parameters 959
simulation of cytochrome P450cam interaction with substrate 567
study of cathepsin B inhibitor docking 977
study of effect of carbon tetrachloride on subtilisin 485
Molecular modelling
of active site of glutamate-specific endopeptidases 591
of bovine type I collagen microfibril 43
of constrained calcitonin gene-related peptide analogues 143
of ligand–receptor interaction 149
of signal peptide function 317
of *Staphylococcus aureus* δ-toxin ion channels 161
Monoclonal antibodies
Fv fragment inhibits cytokine binding to interferon-γ receptor 365
Multiple Copy Simultaneous Search
method for functional group mapping of RNase A 773

Neural network
Kohonen algorithm, for protein structure classification 833
Neutral protease
Bacillus subtilis, improving thermostability of 439
Nicotinic acetylcholine receptor
model of transmembrane domain 51
NMR spectroscopy
automated method for cluster analysis of NMR-derived protein structures [Protocol] 1063
for lithostathine structure determination 949
Non-topological threading
new program for 727
Nuclear magnetic resonance
compared with circular dichroism for estimating secondary structure 15
Nucleation
heterogeneous, preventing [Protocol] 927

OmpA
used to display β-lactamase on *Escherichia coli* cell surface 239
δ-Opioid receptor
3D model of 573
Organic solvents
directed evolution to increase enzyme activity in 77
effect of carbon tetrachloride on subtilisin, molecular dynamics study 485
Outer membrane
Escherichia coli, effects of displaying β-lactamase on cell surface 239

Papain
yeast expression of propapain 1055
Papaya proteinase IV
preventing autoprocessing of proenzyme 525
Pardaxin
derived antibacterial peptides 1219
Penicillium camembertii
lipase, thermostability, effect of inserting disulfide bond 789
Pepsin
Rhizomucor pusillus, catalytic mechanism of 869
Peptide fragments
complementary, for elucidating protein folding pathways 843
Peptidyl–prolyl isomerase
FKBP12, effects of active site mutation 173
Periplasmic degradation
of barnase, effect of altered thermostability 1197
Peroxynitrite
effect on glutathione reductase 189
Phage display
directed selection of antibody repertoires displayed on phage 1043
for analysing HyHEL-10 antibody–antigen interaction 1211
Phosphate binding
by thymidylate synthase, effect of site-directed mutagenesis 69
Phosphoglycerate kinase
yeast model of PGK Uppsala 181
Phospholipase A_2
incorporation of 1,2,4-triazole-3-alanine into active site 345
Pregnancy-associated glycoproteins
comparative modelling of 849
Proenzyme
of papaya proteinase IV, preventing autoprocessing of 525
Profilin
secondary structure analysis of profilin–β-actin complex 1103
Propapain
yeast expression of 1055
Prostaglandin D synthase
glutathione-independent, molecular evolution of [Review] 1067
Protease
HIV-1, binding of inhibitors to 767
Protease activity
screening for following random mutagenesis 85
Protease inhibitors
Cucurbita maxima trypsin inhibitor I, synthesis as fusion protein 1241
efficient production of SLPI C-terminal domain in *Escherichia coli* 101
Protein classification
based on blocks of amino acids 381
Protein contact prediction
by multiple sequence alignment 941
Protein folding
ferredoxin peptide fragment forms native-like β-hairpin 559
lattice model of 5, 387, 399
of human complement receptor 1 SCR1–3 domains 877
pathways of, elucidating using complementary peptide fragments 843
Protein stability
of camelized human V_H domains, improving 531
of *Escherichia coli* tryptophan synthase, role of cysteine residues 425
predicting stability of mutant proteins by mean force-field calculation 479
Protein surface
charge clusters on surface of γ-crystallin 745
hydrophobic patches on, defining from hydration shell structure 1121
Proteinase
HIV-1, linked dimer, effect of mutating active site 997
β-Proteins
comparison of proteins with β-prism architecture 727
structure prediction 399
Prothrombin
introducing fluorescent label into 545
recombinant human, activation by snake venom 921
Prourokinase
chimeric derivatives with thrombin-inhibitory potential 213
Pseudomonas aeruginosa
exotoxin A, for delivering large proteins into cells 611
Pyruvate kinase
mutant favours T conformation 1203

Random mutagenesis
directed evolution of subtilisin E 77
of *Eco*RV DNA methyltransferase 413

screening for protease activity following 85
Rate-determining step
of aldolase, changed by site-directed mutagenesis 61
Reactive site loop
of maspin 585
Receptor binding
of IGF-1, effect of site-directed mutagenesis 1011
Recombinant proteins and peptides
detecting using coiled coil fusion tag 1029
Renaturation
of reduced immunoglobulin G *in vitro* 95
of reduced lysozyme, effect of additives 461
Restriction–modification
structure prediction of *Eco*RV DNA methyltransferase 413
Restriction endonucleases
chimeric, towards the design of 603
*Eco*RV, altering substrate specificity by site-directed mutagenesis 1005
Retroprotein
of *Staphylococcus aureus* protein A, protein folding 5
Rhizomucor pusillus
pepsin, catalytic mechanism of 869
Rhizopus oryzae
lipase, identifying residues important in catalysis 507
Ribonuclease A
functional group mapping of 773
Ribonuclease HI
Escherichia coli, site-directed mutagenesis and X-ray crystallography 857
Ricin
galactose binding by, mutational analysis of 371
ricin–IL-2 fusion toxin 913
R.m.s. distance
as measure of structural similarity 1093
R–T states
pyruvate kinase mutant favours T conformation 1203

'Salting out'
of *Escherichia coli* glutamine synthetase, is abolished by single amino acid substitution 291
Schiff base formation
becomes rate-determining step in engineered aldolase 61
SCR1–3 domains
of human complement receptor 1, folding of 877
Secondary structure
of peptides, estimating using CD and NMR 15
predicting long-range hydrogen bonding from amino acid sequence 133
Self-consistent molecular field theory
applied to structure prediction 387, 399
Semi-empirical simulation
of Zn/Cd binding site preference in metallothionein 1165
Sequence alignment
multiple, for protein contact prediction 941
reliability of 127
Sequence comparison
of theta class glutathione transferases 327
using amino acid similarity matrix 27
Serine proteases
molecular modelling of active site and specificity pockets 591
Serpins
homology modelling of maspin 585
Short consensus repeats
in human decay-accelerating factor 1143
Side-chain–side-chain interaction
role in stability of α-helices 471
Signal peptide
molecular modelling of function 317
Signal transduction
receptor-mediated, evidence that MIF is a trimer 631
Similarity matrix
amino acid, use for sequence comparison and structure prediction 27
for structure classification, constructed by neural network 833
Site-directed mutagenesis
effect on thymidylate synthase phosphate binding 69
engineering disulfide bonds in interferon-γ 905
for altering substrate specificity of *Eco*RV 1005
for altering thermostability, analysis of mutants in a database 265
identifying residues important in catalysis by lipases 507
of aldolase, changes rate-determining step 61
of antibody–antigen interaction 539
of *Escherichia coli* ribonuclease HI 857
of *Escherichia coli* tryptophan synthase 425, 433
of FKBP12 peptidyl–prolyl isomerase 173
of *Humicola lanuginosa* lipase, effect of substrate specificity 519
of HyHEL-10 1211
of IGF-1, effect on receptor binding 1011
of Leu15 in epidermal growth factor, effect on ligand–receptor interaction 781
of maltodextrin phosphorylase 701
of *Rhizomucor pusillus* pepsin 869
of *Sulfolobus solfataricus* β-glycosidase 1191
of *Trichoderma reesei* cellobiohydrolase active site 691
study of cytochrome b_5 interaction with cytochrome *c* 555
to alter thermostability of superoxidase dismutase 323
SLPI
efficient production of C-terminal domain in *Escherichia coli* 101
Snake venom
activates recombinant human prothrombin 921
Specificity pockets
of serine proteases, molecular modelling 591
Stability
effect of Ile96→Ala mutation on stability 273
Staphylococcus aureus
protein A retroprotein 5
δ-toxin ion channels, molecular modelling of 161
Streptavidin
core, fusion with Fv fragment single chain 203
Stress-related proteins
sequence similarities to consensus for theta class glutathione transferases 327
Structure classification
by neural network 833
Structure comparison
by pairwise iterative superposition 1093
detecting non-topological motifs 1103
new program for 727
of glutathione synthetase with other proteins 1083
of MHC class I molecules 1151
Structure determination
of lithostathine, using NMR spectroscopy 949
of yeast model of PGK Uppsala 181
Structure prediction
application of self-consistent molecular field theory 387, 399
*Eco*RV DNA methyltransferase 413
homology modelling of interleukin-7 complex with receptor 1135
of interleukin-7, by homology modelling 493
of thermostable *Escherichia coli* 3-isopropylmalate dehydrogenase 663
predicting leucine zippers from sequence 657
predicting long-range hydrogen bonding from amino acid sequence 133
using amino acid similarity matrix 27
using distance distributions 733
Substrate specificity
of *Eco*RV restriction endonuclease, altering by site-directed mutagenesis 1005
of *Humicola lanuginosa* lipase, effect of site-directed mutagenesis 519
of rat kallikrein rK9, homology modelling 987
Subtilisin
effect of carbon tetrachloride 485
Subtilisin E
directed evolution in *Bacillus subtilis* 77
Subunit dimerization
construction of bacterial luciferase β-subunit hybrids 803
Sulfolobus solfataricus
β-glycosidase, identifying residues essential for catalysis 1191
Superoxidase dismutase
altering thermostability using site-directed mutagenesis 323
SwissProt
protein classification based on blocks of amino acids 381

TAG72 antigen
interaction with B72.3 antibody, site-directed mutagenesis study 539
Thermolysin-like protease
Bacillus stearothermophilus, factors affecting autolysis of 1181
Thermostability
active site of thermostable *Taq* carboxypeptidase 467

altering by site-directed mutagenesis 265
homology modelling of thermostable 3-isopropylmalate dehydrogenase 663
of *Aspergillus awamori* glucoamylase, effect of Glu→Ala mutations 499
of *Bacillus stearothermophilus* thermolysin-like protease, factors affecting 1181
of *Bacillus subtilis* neutral protease, improving 439
of barnase, effect on rate of proteolysis 1197
of enzymes [Forum] 629
of interferon-g, site-directed mutagenesis to improve 905
of superoxidase dismutase, altering using site-directed mutagenesis 323
Penicillium camembertii lipase, effect of inserting disulfide bond 789
Threading method
of structure prediction, applied to β-proteins 399
Three-helix bundle
of retroprotein 5
Thrombin
chimeric derivatives of prourokinase with thrombin-inhibitory potential 213
Thymidylate synthase
effect of site-directed mutagenesis on phosphate binding 69
Tissue-type plasminogen activator
locating unpaired cysteine residue 283
Topological equivalence
defining 1093
δ-Toxin
Staphylococcus aureus, molecular modelling of ion channels 161
T⟷R transition
in insulin hexamer, simulation of 113
Transmembrane domain
algorithm for recognizing in integral membrane proteins 253
of nicotinic acetylcholine receptor, model of 51
of d-opioid receptor, 3D model 573
Trichoderma reesei
cellobiohydrolase, site-directed mutagenesis of active site 691
Trp repressor
semisynthetic scission reagent derived from 603
Trypsin inhibitor
Cucurbita maxima trypsin inhibitor I, synthesis as fusion protein 1241
Tryptophan synthase
Escherichia coli, role of cysteine residues in enzyme function 433
Escherichia coli, role of cysteine residues in stability 425
Tyrosine residues
are target of peroxynitrite modification of glutathione reductase 189

UH-301
molecular modelling of interaction with 5-hydroxytryptamine 1a receptor 149
Unnatural amino acids
incorporation of 1,2,4-triazole-3-alanine into phospholipase A_2 active site 345

V_H domains
camelized human, improving stability of 531

X-ray crystallography
of *Escherichia coli* ribonuclease HI 857
of rat monoclonal Fab against human interleukin-5 623
X-ray diffraction
study of macrophage migration inhibitory factor 631

Yeast expression
of propapain 1055